

# LARGE-SCALE ATOMISTIC SIMULATIONS OF SHOCK PROPAGATION IN METALS

**E. M. Bringa**

Lawrence Livermore National Laboratory  
Livermore CA 94551  
ebringa@llnl.gov

“Single crystal” Cu and Al used in experiments have an initial defect distribution that affects the plasticity threshold along the shock Hugoniot. In this work, shock propagation in Cu and Al is examined for different types of defect structures using molecular dynamics simulations. We have considered voids, grain boundaries, dislocation sources and other defects, and studied how the plastic threshold of the material is decreased by the presence of these defects. Results for shocked nanocrystals will also be shown for different grain sizes.

MD shock simulations typically span 10 ps, and therefore plastic deformation in uniaxial shocks appears as 1D deformation along the shock propagation direction [1]. Experiments for Cu [2] indicate that 3D relaxation of the plastic deformation has already occurred after a few nanoseconds, and estimates based on dislocation mobility suggest that this might be achieved in a shorter time ( $\sim 100$  ps) [2]. We will present atomistic shock simulations spanning 200 ps, for a Cu sample with a length close to one micron and including dislocation sources. Comparison to hydrodynamic codes and dislocation dynamics results will also be discussed.

This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48

## References

- [1] E.M. Bringa *et al.*, *Nucl. Inst. Meth. In Phys. Res. B*, v. 202, p. 56, 2003.
- [2] A. Loveridge-Smith *et al.*, *Phys. Rev. Lett.*, v. 86, p. 2349, 2000.